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Low-Energy Properties of a One-dimensional System of Interacting Bosons with Boundaries

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Abstract. – The ground state properties and low-lying excitations of a (quasi) one-dimensional system of longitudinally confined interacting bosons are studied. This is achieved by extending Haldane's harmonic-fluid description to open boundary conditions. The boson density, one-particle density matrix, and momentum distribution are obtained accounting for finite-size and boundary effects. Friedel oscillations are found in the density. Finite-size scaling of the momentum distribution at zero momentum is proposed as a method to obtain from the experiment the exponent that governs phase correlations. The strong correlations between bosons induced by reduced dimensionality and interactions are displayed by a Bijl-Jastrow wave function for the ground state, which is also derived.

The names of Tomonaga and Luttinger are commonly associated with interacting electron systems in one-dimension (1d). The so-called Tomonaga-Luttinger liquids (TLL's) have the remarkable property that their low-energy spectrum is completely exhausted by gapless collective excitations, i.e. there are no quasiparticles resembling the constituent electrons. However, as emphasized by Haldane [1,2], the class of TLL's is broader than the electron systems that have attracted much attention, especially in recent years. In this paper we shall be concerned with 1d systems whose constituent particles are not electrons, but bosonic atoms. A few experimental systems which fit well these requirements are already available: Atomic vapors confined in highly anisotropic traps [3] and the axial phase of ^{4}He absorbed in narrow pores [4] or nanotubes [5] are good examples. The possibility of TLL behavior in trapped vapors has already been discussed in the literature [7,8]. Monien *et al.* [7] have pointed out that the ground state correlations would decay as power laws, while Yip [8] has found that the absorption line-shape would exhibit power-law singularities.

Motivated by recent experiments [3, 4], we have considered the low-energy excitations and ground state properties of *finite* quasi-1d interacting boson systems. It is important to realize that so far the experimental samples are mesoscopic in size [9] and longitudinally confined. The experimental consequences of this fact for interacting 1d *bosons* have not been fully addressed before. Nevertheless, it is known [10, 11] that the low-energy spectrum and correlation functions of a finite *fermionic* TLL with open boundaries are very different. In

contrast to a system well described with periodic boundary conditions, such as a quantum degenerate gas in a tight toroidal trap (a "boson ring"), a bounded fluid cannot sustain quantized persistent flows, as a ring would, and its excitations are standing waves. Even more important, Eggert *et al.* [11] have shown that the exponents governing correlations in a finite bounded fermionic TLL cross over very slowly to the exponents of the infinite system. The differences illustrate the effect of boundaries on the quantum critical fluctuations characteristic of these systems at very low temperatures, and as we shall argue, they should be taken into account when confronting the experiment. Before we proceed any further, it should be noted that in this letter the longitudinal confining potential is approximated by two infinite barriers at the boundaries. This is not generally the case in current experiments with trapped atomic vapors, where the confining potential is usually harmonic. Accounting for this fact within the formalism employed in this paper is not a difficult task and does not substantially modify the results reported here. Because of space limitations, the necessary modifications to account for slowly varying potentials will be presented elsewhere [30]. However, it is worth pointing out that in recent experiments [6] using microchip traps the confining potential could be tailored to a shape very close to that of a square well with very high barriers. Thus we expect that our results are directly relevant to future experiments in that type of traps, as well as to the ^{4}He systems considered in Refs. [4, 5].

To study the low-energy behavior of a bosonic 1d *quantum* liquid, we rely on Haldane's harmonic-fluid approach [2]. How to generalize this approach to deal with boundaries is explained below. In general, this method is able to account for the long wave-length properties of the system. In this particular case, this means that we cannot describe the properties very close to the boundaries, but for most experiments this is not as important as the effect of the boundaries on the bulk properties. With these provisos, the low-energy effective Hamiltonian as well as asymptotic expressions for the ground state density and one-particle density matrix will be derived in this letter. We also analyze finite-size and boundary effects on the momentum distribution. This quantity is experimentally accessible [16, 17]. Finally, we show that the quadratic character of the effective Hamiltonian allows us to derive Bijl-Jastrow wave function for the ground state [18]. Numerical evidence (e.g. Ref. [13]) suggests that our results should apply to systems containing even a few tens of particles.

We begin by assuming that the system is confined by a very anisotropic potential and that temperature is much lower than the excitation gap for the transverse degrees of freedom (a more detailed analysis of the conditions for (quasi) one-dimensionality can be found in [7, 8, 4, 5, 14, 15]). N_o spinless bosons in the lowest transverse level of the confining potential will be described by the following Hamiltonian,

$$H = \frac{\hbar^2}{2M} \int_0^L dx \, \partial_x \Psi^\dagger(x) \partial_x \Psi(x) + \frac{1}{2} \int_0^L dx \int_0^L dx' \, v(x - x')\rho(x)\rho(x'), \qquad (1)$$

where M is boson mass, $\rho(x) = \Psi^\dagger(x)\Psi(x)$ is the density operator, and $[\Psi(x), \Psi^\dagger(x')] = \delta(x - x')$, but otherwise commute as corresponds to bosons. The interaction $v(x)$ can be totally general as long as it has a short-range repulsive part, and it does not decay slower than $1/|x|^2$. Confinement in the longitudinal direction, x, is described by imposing that the field operator vanishes at the boundaries, i.e. $\Psi(x) = 0$ for $x = 0, L$, where L is the system size. As discussed above, apart from this effect, the longitudinal confining potential is neglected in what follows.

For $v(x) = g \, \delta(x)$ the model was exactly diagonalized by Lieb and Liniger [19]. Lieb [20] also showed that the low-energy excitation spectrum for $g > 0$ is adiabatically connected with that of a system of impenetrable bosons (the Tonks gas [21], where $g \to +\infty$). Girardeau [22]

had previously found that the Tonks gas and a system of free spinless fermions have the same spectrum. The latter presents a Fermi "surface" consisting of two points, and the excitations are particle-hole pairs. The collective modes that exhaust the low-energy spectrum correspond to coherent superpositions of particle-hole pairs. Quite generally, a sufficiently short-ranged potential will make particles effectively impenetrable when their relative energy is small. Therefore, it seems reasonable to expect that the description in terms of the collective modes remains good for a fairly large class of models. Yet, different models have different high-energy structure and this also leads to sizable corrections to the sound velocity and long-distance correlations of the Tonks gas.

To make the discussion more quantitative, we follow Ref. [2] and work in the density-phase representation of the boson field operator, $\Psi^\dagger(x) = \sqrt{\rho(x)}\, e^{-i\phi(x)}$, where $[\rho(x), e^{-i\phi(x')}] = \delta(x - x')\, e^{-i\phi(x)}$. At low energies the matrix elements of $\partial_x \phi(x)$, as well as deviations of $\rho(x)$ from the mean density ρ_o $(\equiv N_o/L)$, are small. Thus, if the long wave-length density fluctuations are represented as $\rho_o + \Pi(x)$, one has $[\Pi(x), \phi(x')] = i\delta(x - x')$, i.e. the fields $\Pi(x)$ and $\phi(x)$ are canonically conjugate. The Hamiltonian in Eq. (1) can be linearized in terms of them to obtain an effective low-energy Hamiltonian,

$$H_{\text{eff}} = \frac{\hbar v_s}{2} \int_0^L dx \left[\frac{\pi}{K}\Pi^2(x) + \frac{K}{\pi} \left(\partial_x \phi(x) \right)^2 \right],$$ (2)

where v_s and K should be regarded as phenomenological parameters. They can be determined either from an exact solution [2, 23] (when available [19, 20]), numerically [13], or from the experiment [4]. Once these parameters have been obtained, the above Hamiltonian provides a complete description of the low-lying excitations, independently of the details of $v(x)$ [1].

Next, we introduce another field $\theta(x)$ related to $\Pi(x)$ by $\partial_x \theta(x)/\pi = \rho_o + \Pi(x)$, which implies that $\theta(x)$ increases by π every time x surpasses one particle. This means that

$$\frac{1}{\pi}\left[\theta(L) - \theta(0)\right] = N$$ (3)

counts the total number of particles in the system. Identifying particle positions with the points where $\theta(x)$ changes by π also allows to construct a representation of the full density operator [2], $\rho(x) = \partial_x \theta(x) \sum_{n=-\infty}^{+\infty} \delta(\theta(x) - n\pi)$, which with the help of Poisson's summation formula can be written as

$$\rho(x) = [\rho_o + \Pi(x)] \sum_{m=-\infty}^{+\infty} e^{2im\theta(x)}.$$ (4)

The field operator is then given (up to an overall prefactor [2]) by

$$\Psi^\dagger(x) \sim [\rho_o + \Pi(x)]^{\frac{1}{2}} \sum_{m=-\infty}^{+\infty} e^{2im\theta(x)}\, e^{-i\phi(x)}.$$ (5)

This expression yields an operator that commutes at different points, as can be checked by using the mode expansions given below. An anti-commuting operator, which represents a Fermi field, can be constructed [2] as $\Psi_F^\dagger(x) = \Psi^\dagger(x)e^{i\theta(x)}$. The above expressions, Eqs. (2) to (5), provide us with the tools to compute the spectrum and correlation functions. However, we have not yet touched upon the issue of boundary conditions. For open boundary conditions (OBC's) we must demand that the field operator vanishes at the boundary, which implies that

$$\sum_{m=-\infty}^{+\infty} e^{2im\theta(0)} = 0.$$ (6)

By construction, this is so if $\theta(0) = \theta_{\mathrm{o}} \neq n\pi$, n being an integer (the precise value of real number $\theta_{\mathrm{o}} \neq n\pi$ will not be important in what follows); The boundary condition is also obeyed for $x = L$ since Eq. (3) relates $\theta(L)$ to $\theta(0)$. The following mode expansions for $\theta(x)$ and $\phi(x)$ are then obtained ($q = m\pi/L$, for $m = 1, 2, 3, \ldots$)

$$\theta(x) \;=\; \theta_{\mathrm{o}} + \frac{\pi x}{L} N + i \sum_{q>0} \left(\frac{\pi K}{qL}\right)^{\frac{1}{2}} e^{-\alpha q/2} \sin(qx) \left[b(q) - b^\dagger(q)\right], \tag{7}$$

$$\phi(x) \;=\; \phi_{\mathrm{o}} + \sum_{q>0} \left(\frac{\pi}{qLK}\right)^{\frac{1}{2}} e^{-\alpha q/2} \cos(qx) \left[b(q) + b^\dagger(q)\right], \tag{8}$$

which diagonalize the Hamiltonian in Eq. (2):

$$H_{\mathrm{eff}} = \sum_{q>0} \hbar\omega(q)\, b^\dagger(q)b(q) + \frac{\hbar\pi v_s}{2LK}(N - N_{\mathrm{o}})^2, \tag{9}$$

where $\omega(q \ll \rho_{\mathrm{o}}) = v_s\, q > 0$, and $[b(q), b^\dagger(q')] = \delta_{q,q'}$, commuting otherwise. That is, the low-energy excitations are linearly dispersing standing "phonons". The cutoff $\alpha \sim \rho_{\mathrm{o}}^{-1}$ in Eqs. (7,8) makes explicit that these expansions are only meaningful as long as we restrict ourselves to a low-energy subspace where the phonon wave-length is much longer than ρ_{o}^{-1}. Besides the phonons, one can create excitations that change the number of particles. These are described by a pair of operators (N, ϕ_{o}), which obey $[N, e^{-i\phi_{\mathrm{o}}}] = e^{-i\phi_{\mathrm{o}}}$. In contrast to PBC's, which were used in [2], only one pair of these operators is needed because, as mentioned in the introduction, one cannot excite quantized persistent flows in a longitudinally confined system. Finally, from Eq. (9) it follows that the compressibility $\kappa = \rho_{\mathrm{o}}^{-2}(d\rho_{\mathrm{o}}/d\mu)$ is proportional to K. The Tonks gas has $K = 1$ (free spinless fermions), while for weakly interacting bosons $K \to +\infty$.

Using Eqs. (4,7) we have computed the ground state density for separations from the boundaries larger than ρ_{o}^{-1}. To leading order in each harmonic of $2\pi\rho_{\mathrm{o}}$ we obtain

$$\langle \rho(x) \rangle = \rho_{\mathrm{o}} \left\{ 1 + \sum_{m=1}^{+\infty} A_m \frac{\cos(2m\pi\rho_{\mathrm{o}}x + \delta_m)}{[\rho_{\mathrm{o}}d(2x)]^{m^2 K}} \right\}, \tag{10}$$

where $d(x) = (2L/\pi)\left|\sin(\pi x/2L)\right|$, and A_m and δ_m are model dependent coefficients [24]. Since in 1d the distinction between bosons and fermions is blurred by interactions [2], the ground state density exhibits Friedel oscillations characteristic of Fermi systems [10, 12, 13]. They are induced by the boundaries, which break translational symmetry, and therefore would be absent if we had assumed PBC's. For sufficiently strong repulsive interactions ($K < 2$ [2, 25, 30]), these oscillations can be pinned by a periodic potential (e.g. an optical lattice) of wave length equal to ρ_{o}^{-1}. The system would thus undergo a transition to a Mott insulating regime [26].

The presence of the boundaries also modifies the structure of correlation functions. We have computed the one-particle density matrix at zero temperature. Far from the boundaries and for $|x - x'| \gg \rho_{\mathrm{o}}^{-1}$, the result reads

$$\langle \Psi^\dagger(x)\Psi(x') \rangle \;\sim\; \rho_{\mathrm{o}} \left[\frac{\rho_{\mathrm{o}}^{-1}\sqrt{d(2x)d(2x')}}{d(x+x')d(x-x')} \right]^{\frac{1}{2K}} \sum_{m,m'=-\infty}^{+\infty} C_{m,m'}\, e^{-i(m+m')\pi\,\mathrm{sgn}(x-x')/2}$$

$$\times \left[\frac{d(x+x')}{d(x-x')}\right]^{2mm'K} \frac{e^{2\pi i\rho_{\mathrm{o}}(mx-m'x')}}{[\rho_{\mathrm{o}}d(2x)]^{m^2 K}[\rho_{\mathrm{o}}d(2x')]^{m'^2 K}}. \tag{11}$$

Again $B_{m,m'}, C_{m,m'}$ are model dependent (complex) coefficients which cannot be determined by this method. Bulk behavior is recovered for $|x - x'| \ll \min\{x, x', L - x, L - x'\}$. In this limit, the less oscillatory terms in Eq. (11) are those where $m = m'$, which yield the expression in Ref. [2] [27]. Using the same formalism other correlation functions, such as the density correlation function, have been obtained. These will reported elsewhere [30] as only the density matrix, Eq.(11), is needed here.

From the one-particle density matrix the momentum distribution can be obtained [11]:

$$n(p, L) = \frac{1}{L} \int_0^L dx \int_0^L dx' \, \langle \Psi^\dagger(x) \Psi(x') \rangle \, e^{ip(x-x')}, \qquad (12)$$

which we have normalized so that $(2\pi\rho_o)^{-1} \int dp \, n(p) = 1$. The dominant contribution at small momentum is given by the $m = m' = 0$ term in Eq. (11), henceforth denoted $f(x, x', L)$. In the thermodynamic limit $L \to \infty$, this function decays as $|x - x'|^{-1/2K}$, which implies that $n(p \ll \rho_o) \sim p^{-\beta}$ with $\beta = 1 - (2K)^{-1}$. However, when the system is finite these power laws do not hold. This poses a problem to determine the exponent β from experimental measurements of the momentum distribution. Measuring the exponent is important, not only as a means to obtain K and get an idea of the strength of the interactions, but also because β controls the decay of phase correlations: For β close to 1 (i.e. $K \gg 1$) phase correlations will decay very slowly, and therefore the system will look like a Bose-Einstein condensate, even if, strictly speaking, in 1d bosons do not condense. On the other hand, when $\beta \approx 1/2$, the system will behave as a Tonks gas.
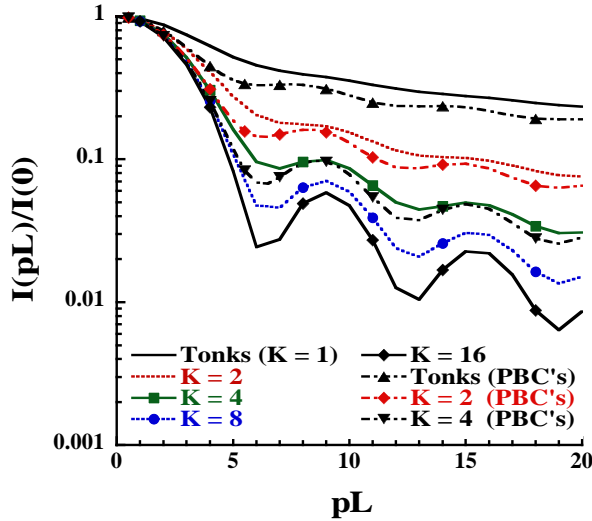

Fig. 1 – Momentum distribution $n(p, L)$ vs. pL (L is the system's size), for different values of K. It has been normalized to its value at $p = 0$ (Recall that $n(0, L) = (\rho_o L)^\beta \, I(0)$, with $\beta = 1 - (2K)^{-1}$. Hence $n(p, L)/n(0, L) = I(pL)/I(0)$, cf. Eq. (13)). Some results ($K = 1, 2, 4$) with periodic boundary conditions (PBC's) are also shown for comparison.

To find the exponent β, we must resort to a different type of analysis. Let us first note that the function $f(x, x', L)$ is homogeneous, i.e. $f(x, x', L) = s^{1/2K} f(sx, sx', sL)$. Choosing $s = 1/L$, it follows that $f(x, x', L) = L^{-1/2K} F(x/L, x'/L)$, for some *scaling* function $F(\xi, \xi')$. Introducing this result into Eq. (12),

$$n(p \ll \rho_{\rm o}, L) = (\rho_{\rm o} L)^{\beta} \ I(pL), \tag{13}$$

where $I(pL) = 2\rho_{\rm o}^{-\beta} \int_0^1 d\xi \int_0^1 d\xi' \ F(\xi, \xi') \cos[pL(\xi - \xi')]$. This function has been plotted in Fig. 1 for different values of K. Eq. (13) thus implies that the exponent β can be extracted from a finite-size scaling analysis of the experimental data for $n(0, L)$ collected in systems of different size but equal density, $\rho_{\rm o}$. Girardeau and Wright [16] have proposed a non-destructive method to measure $n(p, L)$. With this technique, one can try to obtain $n(p \to 0, L)$ as a function of L, using a blue-detuned laser beam to split a quasi 1d trapped atomic gas into pieces of smaller size which could be probed independently. Real systems, however, are at finite temperature, whereas the previous analysis is for $T = 0$. At finite temperature, correlations decay exponentially with distance [1]. Repeating the above analysis $n(p, L, T) = (\rho_{\rm o} L)^{\beta} I'(pL, TL/\hbar v_s)$. Thus, when measuring systems of different size the product TL must be kept constant. However, for $T < \hbar v_s/L_{\max}$, where $L_{\max}$ is the size of the largest system considered, quantum fluctuations dominate over thermal fluctuations and the dependence on T can be neglected so that our $T = 0$ analysis should be valid.

Finally, we derive a Bijl-Jastrow wave function for the ground state of $N_{\rm o}$ interacting bosons confined in a box with open boundaries. For the Tonks gas, it was pointed out by Girardeau [22] that the exact ground state is of Bijl-Jastrow form. Recently, Pham *et al.* [18] have remarked that the quadratic form of the effective Hamiltonian, Eq. (2), implies that a Bijl-Jastrow wave function is a good approximation to the ground state. Here we extend their derivation to OBC's. Expanding $\Pi(x) = \Pi_{\rm o}/L + \sqrt{2/L} \sum_{q>0} \hat{\Pi}_q \cos(qx)$ and $\phi(x) = \phi_{\rm o} + \sqrt{2/L} \sum_{q>0} \hat{\phi}_q \cos(qx)$, with $[\hat{\Pi}_q, \hat{\phi}_{q'}] = i\delta_{q,q'}$ and $\Pi_{\rm o} = N - N_{\rm o}$, $H_{\rm eff}$ is given by

$$H_{\rm eff} = \frac{\hbar \pi v_s}{2K} \sum_{q>0} \left[\Pi_q^2 - \left(\frac{qK}{\pi} \right)^2 \frac{\delta^2}{\delta \Pi_q^2} \right] + \frac{\hbar \pi v_s}{2LK} \Pi_{\rm o}^2, \tag{14}$$

where $\hat{\phi}_q$ has been replaced by $-i\delta/\delta \Pi_q$, as implied by its commutator with $\hat{\Pi}_q$. Thus the ground state is a gaussian in momentum space, $\Phi_{\rm o} = \exp \left\{ -\pi \sum_{q>0} \Pi_q^2/2qK \right\}$, which in real space reads

$$\begin{aligned} \Phi_{\rm o}(x_1, \ldots, x_N) &= \exp \left\{ \frac{1}{2} \int_0^L dx \int_0^L dx' \ \rho(x) \mathcal{K}(x, x') \rho(x') \right\} \\ &\propto \prod_{i=1}^{N_{\rm o}} \left[\frac{d(2x_i)}{\pi^{-1} L} \right]^{\frac{1}{2K}} \prod_{i<j} \left[\frac{d(x_i + x_j) d(x_i - x_j)}{\pi^{-2} L^2} \right]^{\frac{1}{K}}, \end{aligned} \tag{15}$$

where we have replaced $\Pi(x)$ by $\rho(x) - \rho_{\rm o}$, and then used $\rho(x) = \sum_{i=1}^{N_{\rm o}} \delta(x - x_i)$ and $\mathcal{K}(x, x') = \log \left| L^{-2} \pi^2 d(x + x') d(x - x') \right| / K$. The result bears some resemblance to the exact ground states of the Tonks gas [28] ($K = 1$) and the Calogero-Sutherland [29] models in a harmonic trap. The differences are due to the different confining potential considered. As in those cases, however, the wave function vanishes when two particles approach each other, revealing strong correlations between the bosons.

In conclusion, we have extended the harmonic-fluid approach [2] to obtain the low-lying excitations and study finite-size and boundary effects in systems of interacting bosons in 1d that are confined longitudinally. When analyzing their properties, these effects must be taken into account. This has been illustrated by considering the momentum distribution at small momentum, which does not behave as the power law predicted for the infinite system. Finally, we have also derived a Bijl-Jastrow wave function for the ground state. A more complete account will be given elsewhere [30].

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